

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
 Data File : BF127979.D
 Acq On : 28 Apr 2022 14:23
 Operator : CG\JU
 Sample : N2482-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COP-1R

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.069	299	303	309	rVB	142995	180764	3.73%	0.644%
2	4.275	334	338	342	rBV	49500	59015	1.22%	0.210%
3	5.175	486	491	501	rBV	118711	145965	3.01%	0.520%
4	5.557	548	556	559	rBV	2710060	2713614	55.96%	9.666%
5	5.787	591	595	598	rBV	194915	161633	3.33%	0.576%
6	6.551	716	725	733	rBV	2042320	2092448	43.15%	7.454%
7	6.728	752	755	757	rBV	152995	141034	2.91%	0.502%
8	6.757	757	760	773	rVV2	191030	289173	5.96%	1.030%
9	6.851	773	776	786	rVV	184333	289725	5.97%	1.032%
10	6.928	786	789	796	rVB	770137	702200	14.48%	2.501%
11	7.098	815	818	822	rBV2	54768	59985	1.24%	0.214%
12	7.245	840	843	853	rVB4	24948	49553	1.02%	0.177%
13	7.333	853	858	864	rVB3	44418	53968	1.11%	0.192%
14	7.498	880	886	889	rVB	2618269	2845778	58.69%	10.137%
15	7.569	893	898	901	rBV	61947	70176	1.45%	0.250%
16	8.151	988	997	1000	rBV2	66710	99002	2.04%	0.353%
17	8.210	1003	1007	1016	rVB	861063	910946	18.79%	3.245%
18	8.539	1059	1063	1070	rBV3	57401	78151	1.61%	0.278%
19	8.622	1073	1077	1087	rVB	53340	74979	1.55%	0.267%
20	9.204	1172	1176	1182	rBV3	38219	92544	1.91%	0.330%
21	9.292	1185	1191	1194	rBV	4794227	4849197	100.00%	17.274%
22	9.386	1204	1207	1221	rVB	979133	1106732	22.82%	3.942%
23	9.969	1301	1306	1310	rBV	1052990	958664	19.77%	3.415%
24	10.380	1372	1376	1380	rVB2	76338	82793	1.71%	0.295%
25	10.674	1422	1426	1433	rBV2	80885	93284	1.92%	0.332%
26	10.769	1436	1442	1445	rBV	2916447	3013550	62.15%	10.735%
27	11.463	1556	1560	1563	rBV	1123990	952844	19.65%	3.394%
28	11.839	1621	1624	1628	rVB	264904	234280	4.83%	0.835%
29	12.551	1740	1745	1748	rVB2	223996	187498	3.87%	0.668%
30	13.057	1826	1831	1834	rBV	4226274	4250248	87.65%	15.140%
31	14.110	2006	2010	2016	rVB	610439	600540	12.38%	2.139%
32	15.615	2261	2266	2277	rBV	458372	632140	13.04%	2.252%

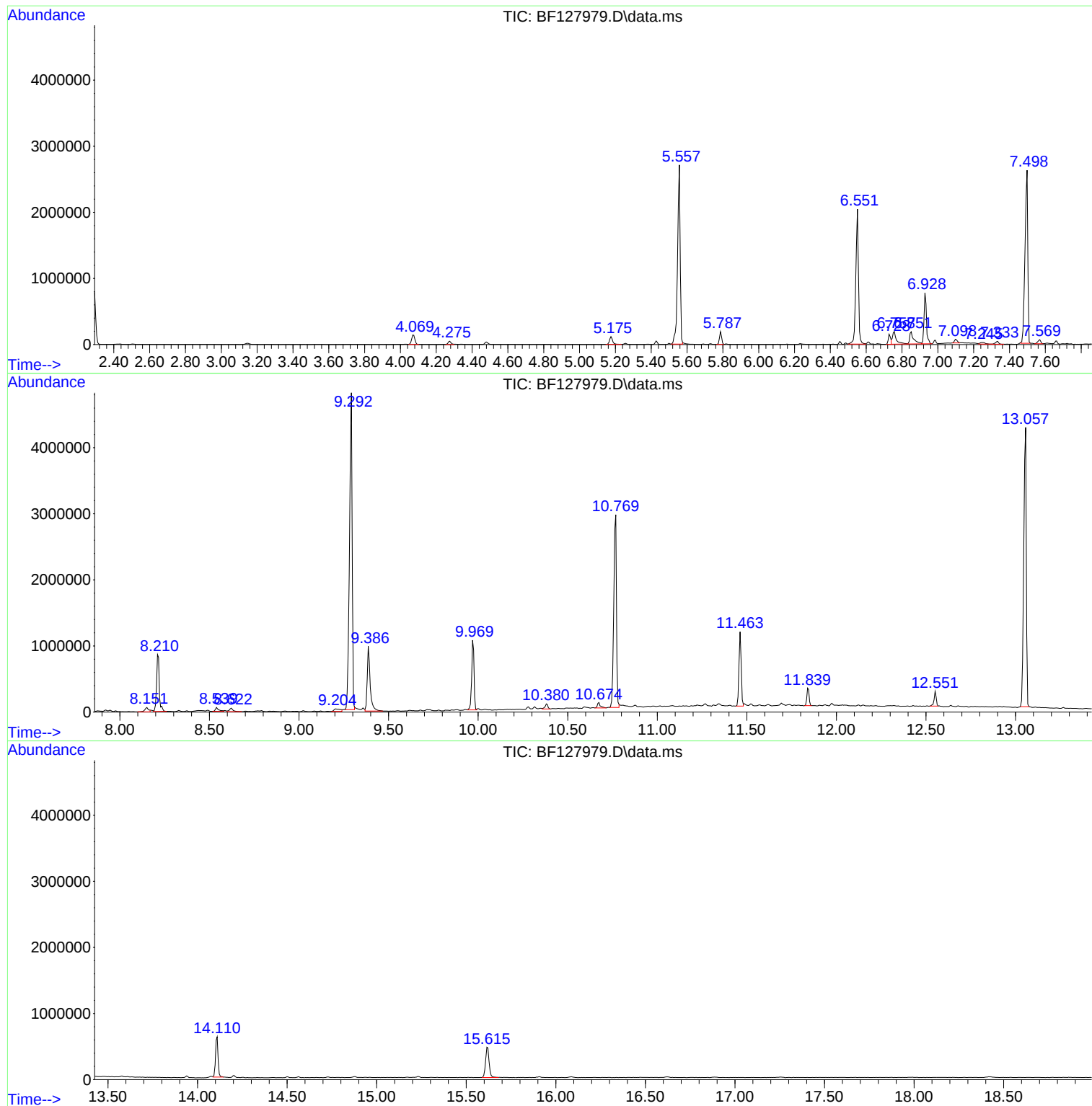
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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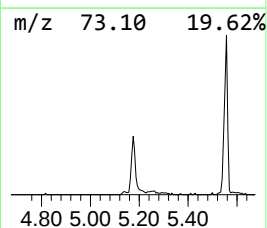
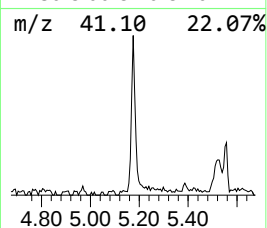
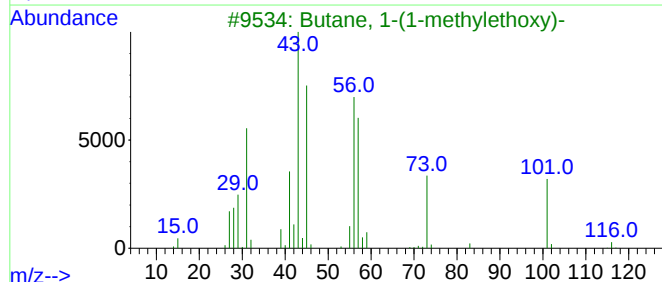
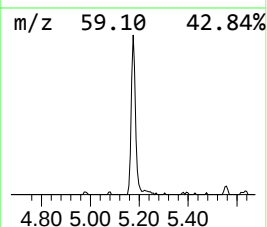
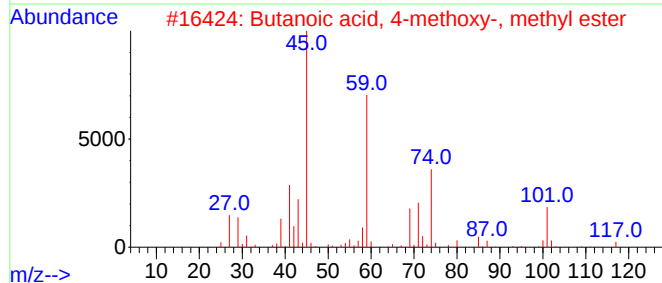
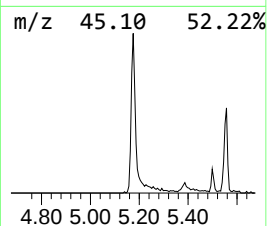
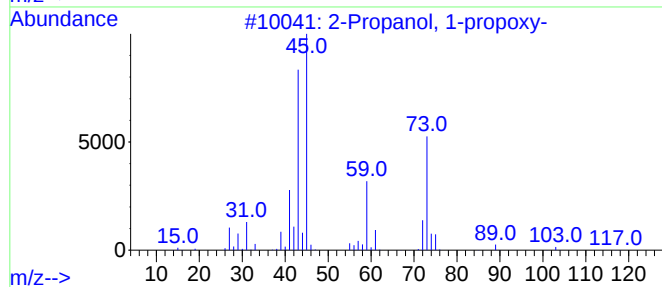
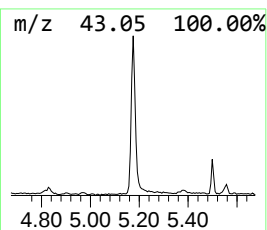
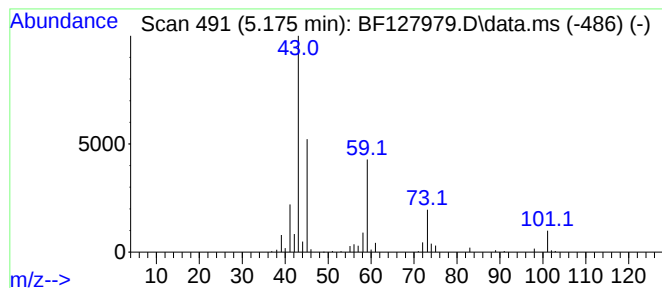
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.175 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	4.16 ng	145965	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-			118	C6H14O2	001569-01-3	43
2	Butanoic acid, 4-methoxy-, methyl ester			132	C6H12O3	029006-01-7	42
3	Butane, 1-(1-methylethoxy)-			116	C7H16O	001860-27-1	38
4	Ethanol, 2-(1-methylethoxy)-			104	C5H12O2	000109-59-1	37
5	Butanoic acid, 4-methoxy-			118	C5H10O3	029006-02-8	28



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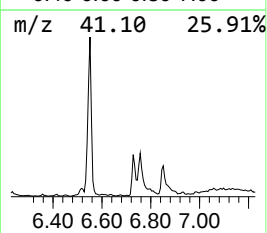
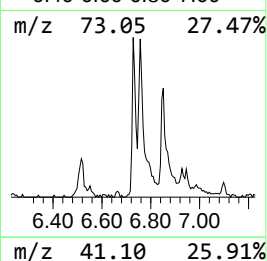
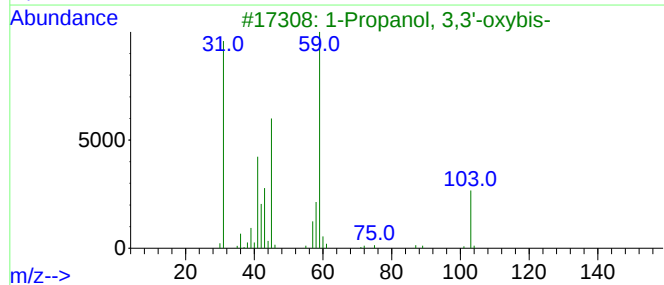
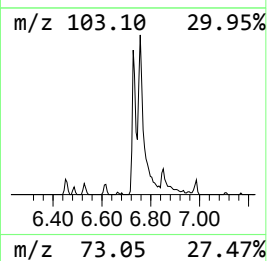
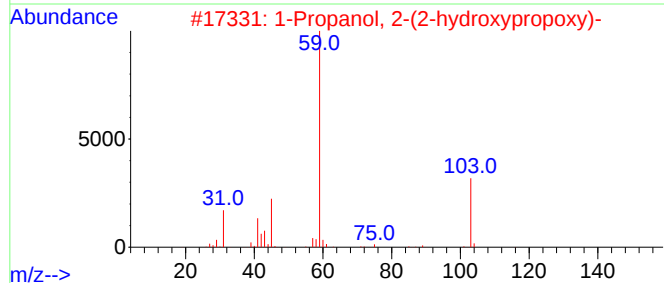
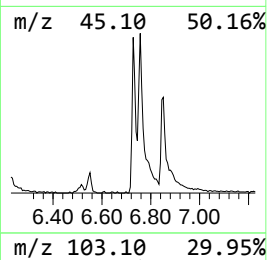
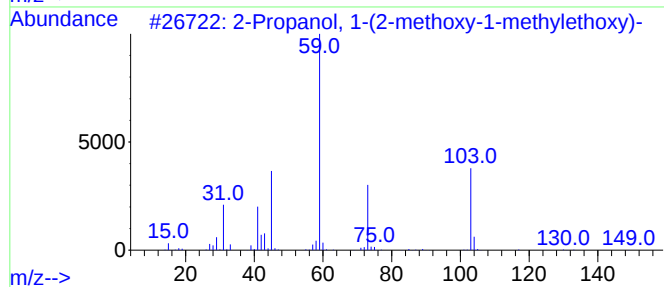
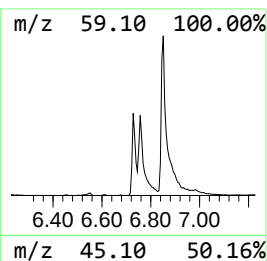
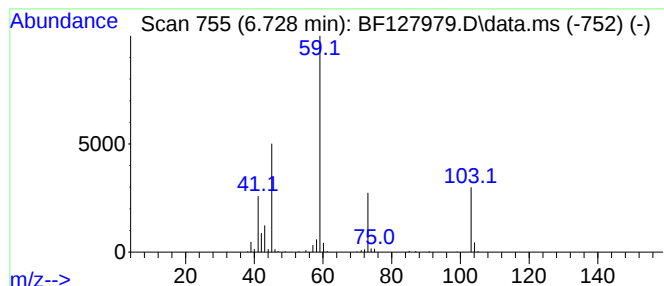
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	4.02 ng	141034	1,4-Dichlorobenzene-d4	6.928

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	80
2		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3		1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	50
4		Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
5		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42



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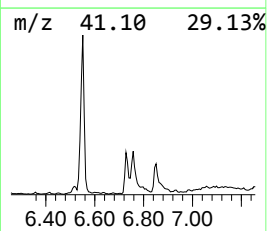
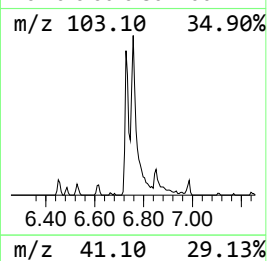
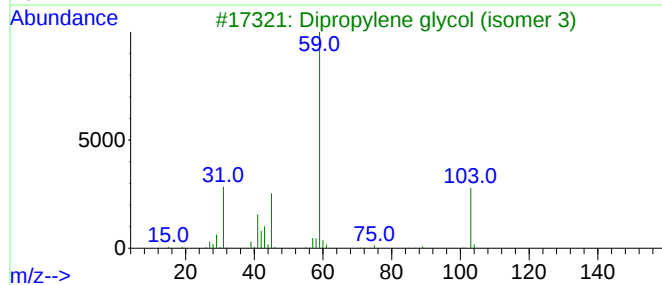
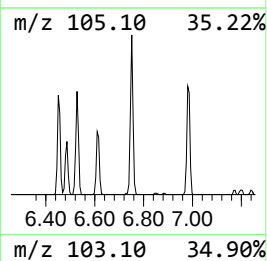
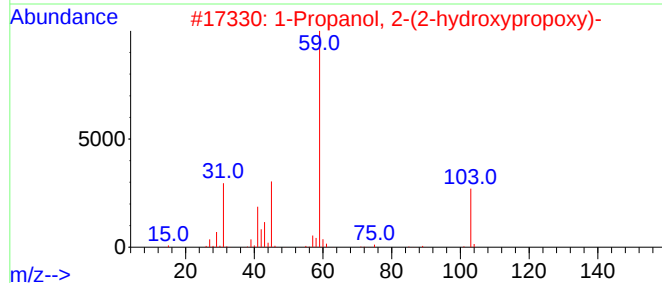
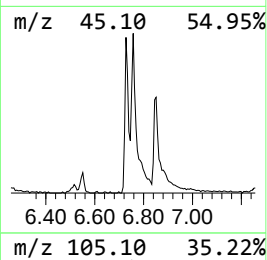
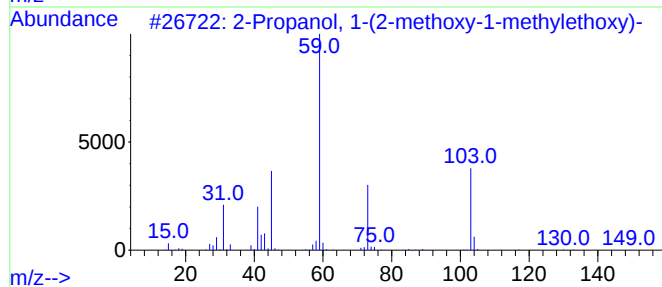
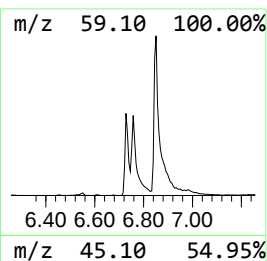
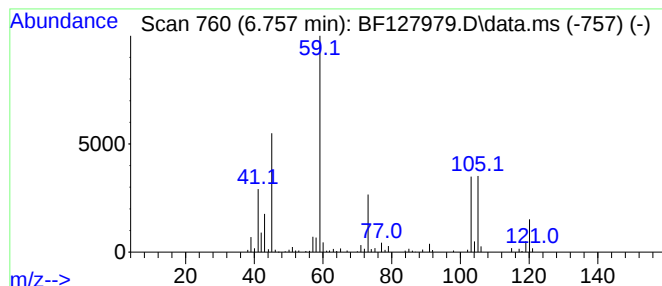
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.757 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.757	8.24 ng	289173	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	58		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	47		
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	47		
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	47		
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	47		



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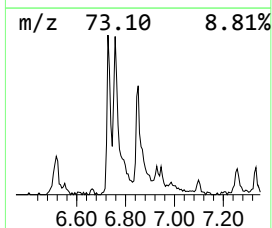
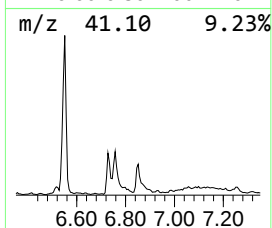
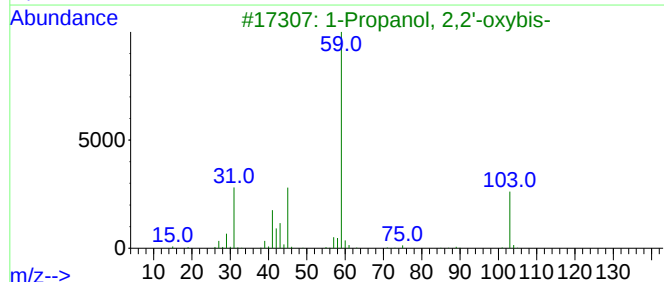
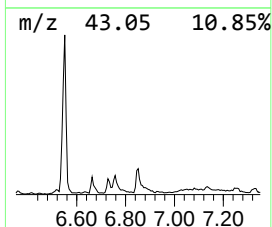
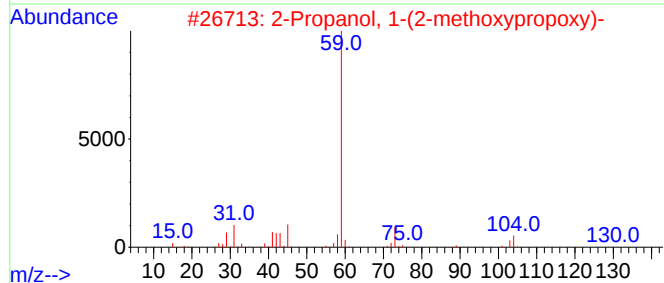
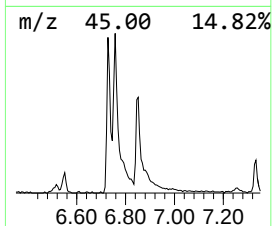
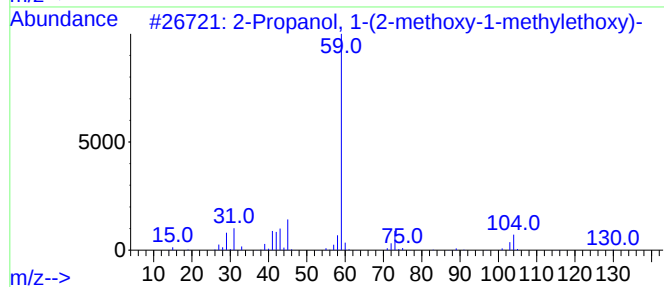
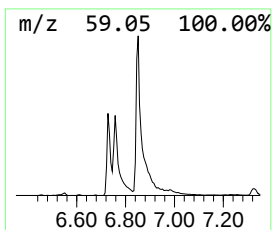
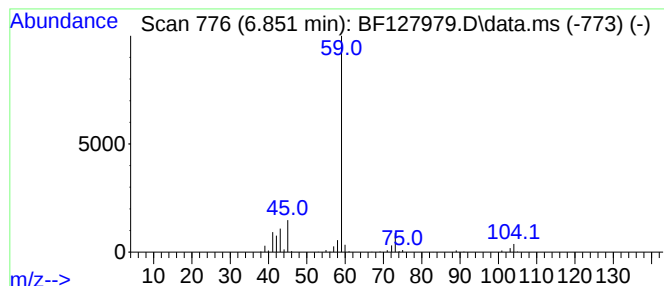
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Peak Number 6 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.851	8.25 ng	289725	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83		
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	78		
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64		



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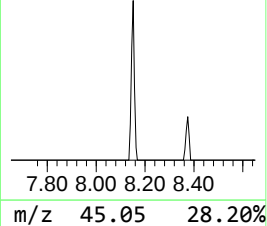
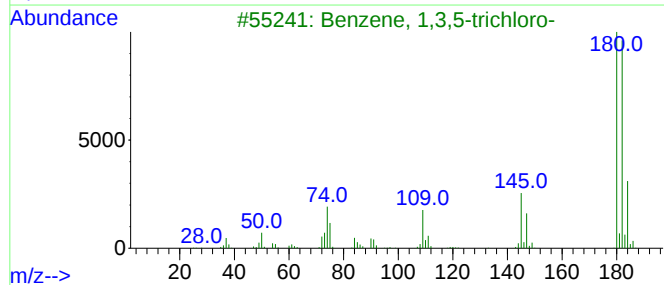
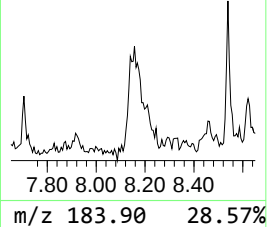
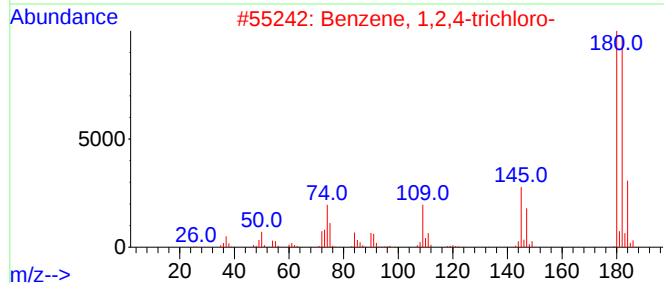
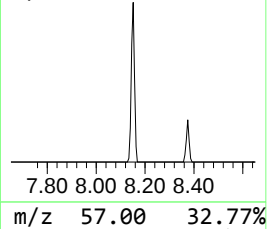
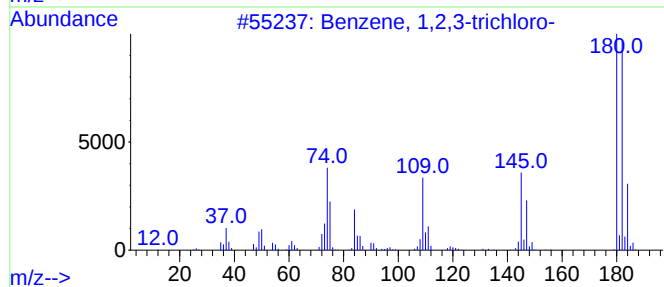
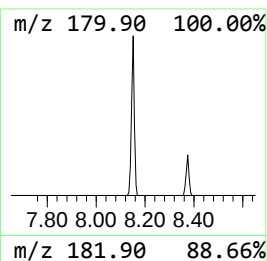
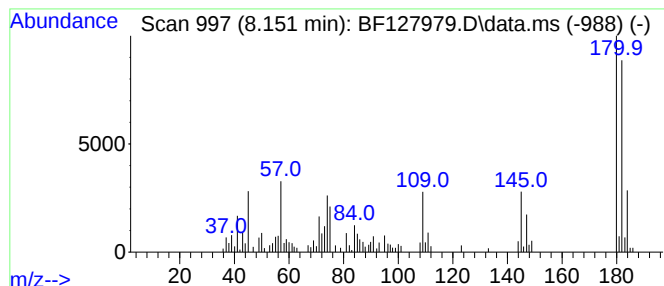
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Peak Number 7 Benzene, 1,2,3-trichloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.151	2.17 ng	99002	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	94
2			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	94
3			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	91
4			4-Bromo-4-chloropyrazole	180	C3H2BrClN2	1000435-93-9	53
5			Benzene, (bromoethynyl)-	180	C8H5Br	000932-87-6	50



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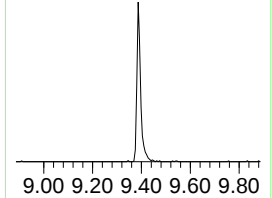
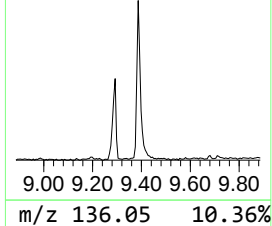
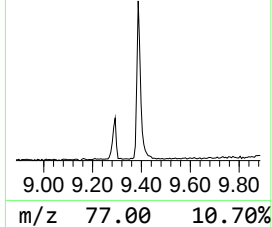
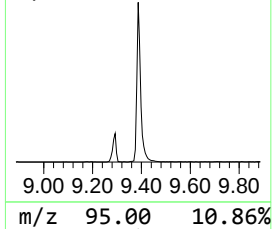
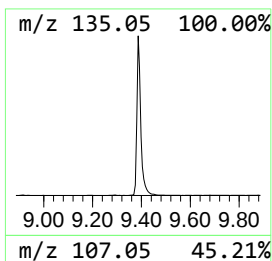
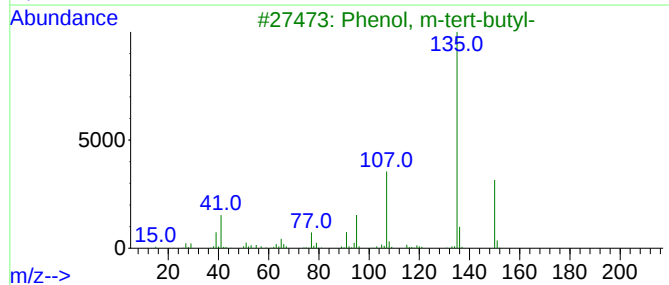
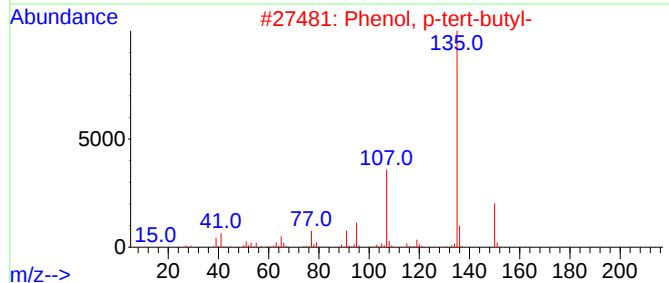
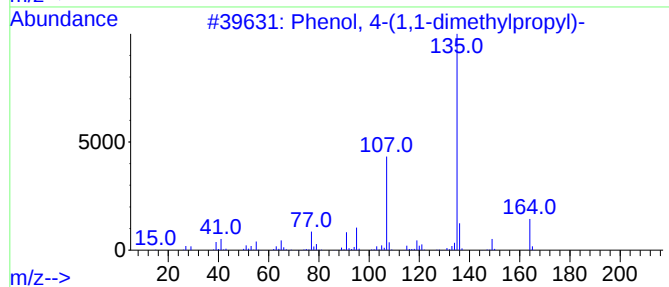
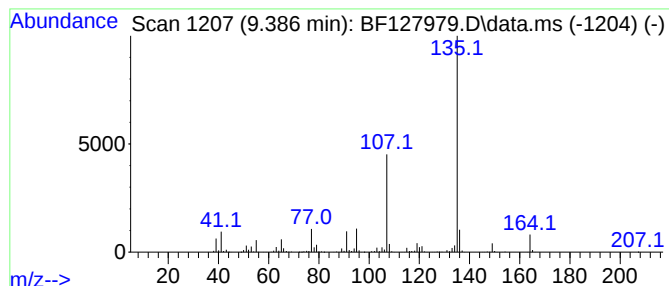
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	23.09 ng	1106730	Acenaphthene-d10	9.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
4		4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5		Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127979.D
Acq On : 28 Apr 2022 14:23
Operator : CG\JU
Sample : N2482-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COP-1R

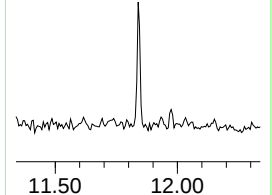
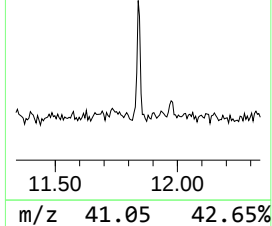
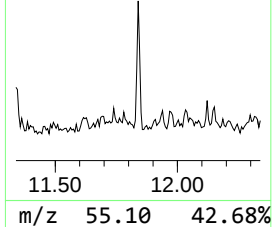
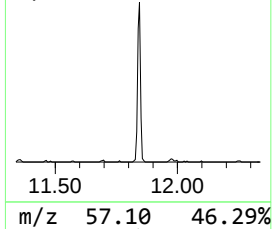
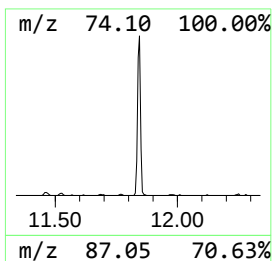
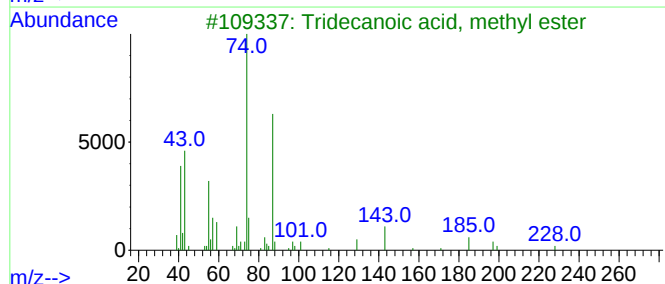
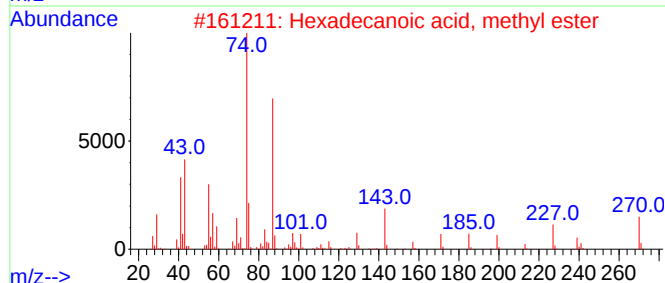
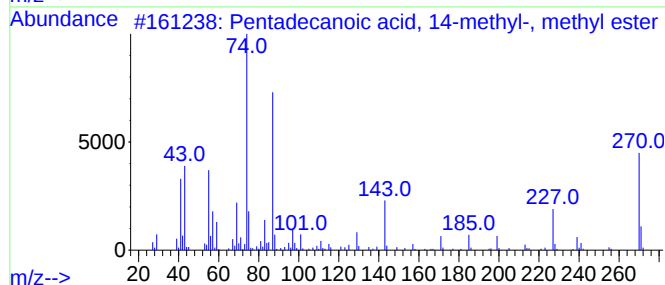
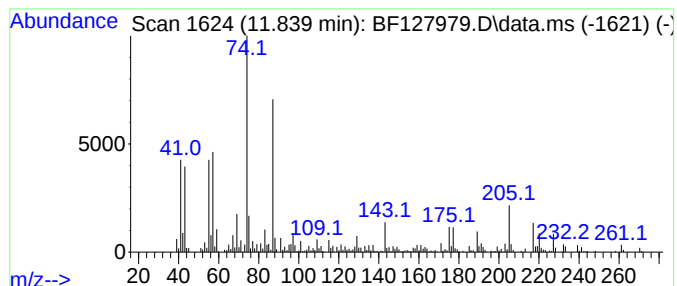
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Pentadecanoic acid, 14-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.92 ng	234280	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	83
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	78
4			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	60
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127979.D
Acq On : 28 Apr 2022 14:23
Operator : CG\JU
Sample : N2482-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COP-1R

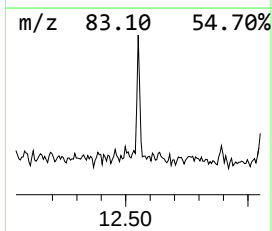
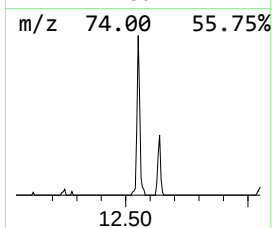
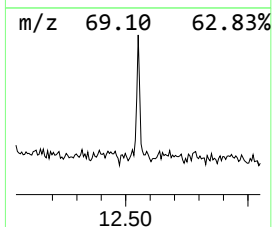
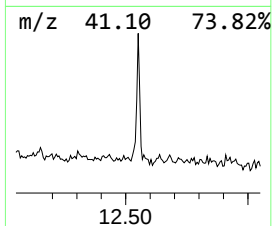
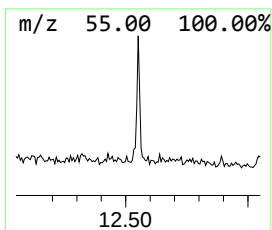
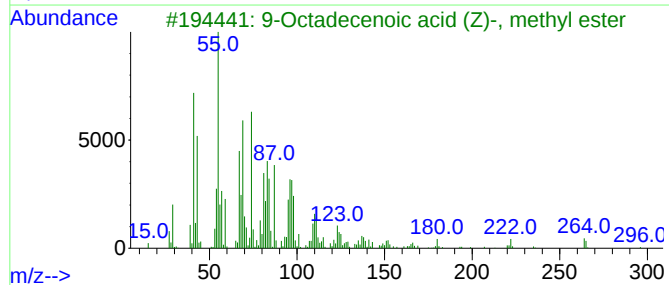
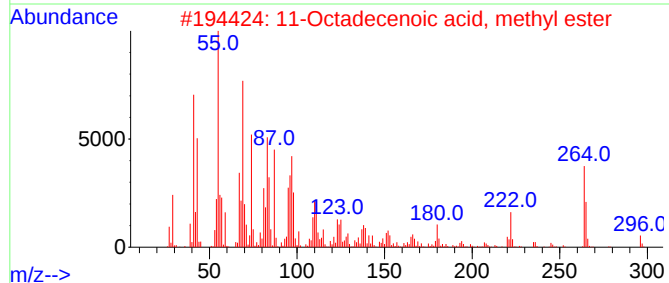
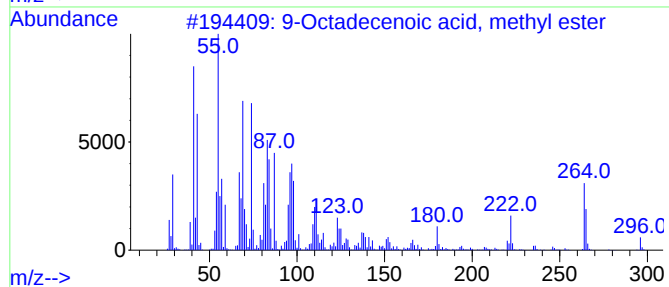
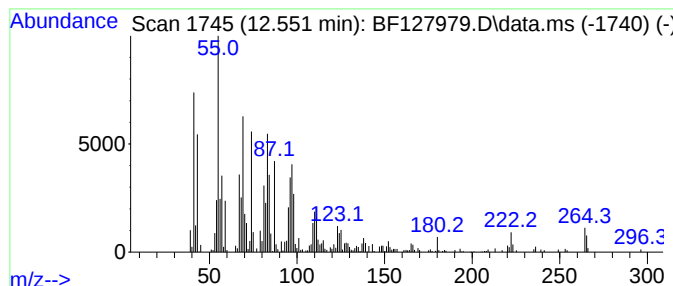
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 9-Octadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	3.94 ng	187498	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
4			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127979.D
Acq On : 28 Apr 2022 14:23
Operator : CG\JU
Sample : N2482-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COP-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.175	5.175	4.2	ng	145965	1	6.928	702200	20.0
2-Propanol, 1-(...	6.728	4.0	ng	141034	1	6.928	702200	20.0
unknown6.757	6.757	8.2	ng	289173	1	6.928	702200	20.0
2-Propanol, 1-(...	6.851	8.3	ng	289725	1	6.928	702200	20.0
Benzene, 1,2,3-...	8.151	2.2	ng	99002	2	8.210	910946	20.0
Phenol, 4-(1,1-...	9.386	23.1	ng	1106730	3	9.969	958664	20.0
Pentadecanoic a...	11.839	4.9	ng	234280	4	11.463	952844	20.0
9-Octadecenoic ...	12.551	3.9	ng	187498	4	11.463	952844	20.0